

From Theory to Simulation: Computational Modelling in Science Education

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Abstract. Computer simulations are increasingly used in STEM classrooms, yet they often remain black-box tools that illustrate settled concepts rather than supporting authentic inquiry. This article examines how computational modelling can bridge disciplinary domain expertise and interdisciplinary STEM skills by making modelling decisions explicit. We combine an expert study with 32 German-speaking STEM didactics and subject-matter researchers, and a case study on the interdisciplinary development of a forest ant locomotion simulation for biology lessons, implemented iteratively in *Snap!*. Expert responses were inductively coded to refine a cross-disciplinary definition of modelling and to identify priority learning goals. The case study traces the full communication and prototyping process (15 prototypes) and analyses 27 modelling decisions, categorised as domain-specific, computer-science related, usability-driven, or pragmatic, including their dependency structure. Across both studies, results highlight the centrality of cyclic revision and reflection, the challenge of terminology mismatches between disciplines, and the ways computational constraints and representations shape domain models. We discuss teaching implications: students need opportunities to create, adapt, and justify simulations (not only use them), supported by explicit vocabulary for modelling decisions and structured collaboration between computer science and science education.

Keywords: Simulation · Computer science · Modelling · STEM

1 Introduction

The ability to analyse and understand complex phenomena through models is a core competency in science, technology, engineering and mathematics (STEM) subjects [1,2]. Modelling enables learners to investigate theoretical concepts behind real-life phenomena and thus develop a deeper understanding of scientific disciplines. Modelling not only contributes to knowledge transfer but also offers an opportunity for active engagement with scientific methods through authentic learning processes. While theory and experimentation have traditionally been considered the central pillars of knowledge acquisition, simulation has established itself as a third pillar of science with the increasing digitisation [3]. Simulations translate theoretical models into dynamic, interactive scenarios and allow phenomena to be investigated, predictions to be made, and hypotheses to be tested, especially when real experiments are not feasible or difficult to carry

out. The creation of such digital models requires computational modelling when preparing and transforming subject-specific problems in a way that they can be carried out by a computational system. Accordingly, computational modelling is also gaining importance beyond computer science. Although simulations are increasingly used in STEM subjects in schools to map complex processes, generate and analyse data, and experimentally investigate scientific phenomena, in practice, such simulations are often limited to ready-made, black-box tools to illustrate well-known concepts. However, a critical approach to simulations requires a deeper understanding: learners should also be familiar with the underlying computational modelling decisions in order to evaluate their effects and, if necessary, further develop simulations. As Peperkorn et al. [4] summarise, “creating one’s own simulation to model a specific system yields a higher learning output compared to using a preprogrammed simulation”.

This research aims to develop approaches for such an interdisciplinary understanding of modelling and to identify challenges in the application of computational modelling competence in the context of simulations in STEM subjects. After presenting the current state of research, a qualitative study is presented in which first experts were surveyed in order to identify a cross-disciplinary understanding of modelling and corresponding learning goals. In a case study on the development of a biology teaching simulation, the results of the computational and subject-specific modelling decisions made were examined in order to relate the findings to their practical implications. Finally, teaching implications for fostering computational modelling in science education are drawn.

2 Related Prior Research

Modelling generally refers to designing a model for a specific purpose based on an observed phenomenon or system in the real world [5]. Modelling is a central scientific practice in all STEM subjects and serves to analyse, structure, and predict complex phenomena [6]. While models in the natural sciences are often used to describe relationships and form hypotheses [7], the focus in computer science education is on computational modelling: the construction and implementation of models [8]. These different perspectives make it difficult to achieve a uniform understanding of modelling and modelling competence in STEM education in schools [9]. Modelling is generally understood as a cyclical process in which models are developed, tested, and adapted iteratively [10]. Two main perspectives can be distinguished. A product-oriented view considers the model as the end product of a modelling process, for example, as a mathematical equation, diagram, or simulation [11]. The process-oriented perspective, on the other hand, focuses on the reflection and iterative adaptation of the model as part of a scientific knowledge process [12]. This distinction is particularly relevant for interdisciplinary modelling, as computer science and natural sciences differ in their understanding of models. While computer science traditionally emphasises a product-oriented perspective in this sense, with models being formally specified and implemented, the natural sciences place greater emphasis on the application perspective, with models being used to form hypotheses and interpret empirical data [13]. Even though simulations are

considered the third pillar of the scientific knowledge process alongside theory and experimentation, this perspective has been underrepresented in school STEM education [14]. Computer science education opens up a new perspective here by focusing on modelling as a conscious process in which modelling decisions are reflected upon and adapted [15].

Krüger and Upmeier zu Belzen [12] distinguish between model competence and modelling competence based on their respective focus and process involvement. Model competence refers to the ability to understand, apply, and critically reflect on existing models. In particular, it includes the analysis of models, their usefulness and limitations, and the interpretation of model assumptions and statements. Model competence is therefore more recipient-oriented and focused on the use of models. Modelling competence, on the other hand, additionally includes the ability to develop, revise, and adapt models oneself. It thus describes an active, creative process in which phenomena from the world of experience are abstracted, structured, and transferred into a model. Modelling competence requires an understanding of model building as a cyclical process in which assumptions are made, hypotheses are tested, and models are iteratively improved. The modelling competence of students is largely determined by whether they not only use simulations, but also understand how they work and the principles of modelling [16]. While science classes in school often focus on the use of ready-made simulation models, in computer science education, the development and implementation of one's own models is central [17]. Studies show that a deep understanding of simulations can only be achieved when learners are able to adapt or expand the models themselves [18]. This is particularly relevant for phenomena that cannot be directly experienced, such as those at the molecular level, where simulations often serve as the sole source of knowledge and must be critically questioned [19]. With appropriate support, students can learn to apply computational modelling to model real-world phenomena in a subject domain and to identify appropriate representations using concepts and abstractions from the computing domain [20].

Based on the previous research, the following general definition of modelling was derived: modelling is a scientific and cyclical method in which models are created and applied for specific purposes. In modelling, the world of experience with its phenomena and empirical investigation for the purpose of obtaining data, and the world of models with theoretical foundations and technical ways of thinking are fundamentally interrelated. Phenomena from the world of experience are analysed and transferred into a model with a specific purpose. This model is applied to investigate phenomena and solve problems in the world of experience.

Despite the relevance of modelling and simulations in STEM education, several desiderata are apparent. On the one hand, there is a lack of interdisciplinary understanding of modelling, as the terms and concepts of modelling are defined differently depending on the discipline, and there have been few attempts to systematically link these perspectives. Second, it remains unclear how computational modelling skills can be integrated into STEM-specific modelling practices, for example, with the goal of enabling learners to adapt or further develop simulations themselves.

3 Research Questions and Methods

This research investigates how computational modelling can contribute to learners' understanding of simulations and their underlying domain models with the aim of developing approaches for a cross-disciplinary understanding of modelling in STEM subjects. Accordingly, we look at both the cross-disciplinary understanding of modelling and its application in the computational modelling process of a STEM simulation:

RQ1: What characterises a cross-disciplinary understanding of modelling in STEM subjects?

RQ2: Which aspects of modelling competence are considered by experts to be of central importance for targeted promotion in STEM education?

RQ3: How are these characteristics reflected in the interdisciplinary development of a scientific simulation?

RQ4: What influences computational modelling as reflected in the relationship between computer science and domain-specific modelling decisions in the interdisciplinary development of simulations?

RQ1 and RQ2 were addressed in an expert study, which was conducted as part of a joint STEM project on the topics of modelling, risk, and uncertainty, whereby only the sub-study on modelling and modelling competence is considered further here. Thirty-two German-speaking experts participated in this study. They were selected on the basis of their professional suitability (STEM didactics/subject science, research focus, or publication on modelling) and qualifications (at least three years after obtaining a doctorate) and were approached by the project network. To this end, the participants were given a theoretically derived definition of modelling and modelling competency, which was developed earlier in the project context and supported by the participating STEM perspectives (biology, computer science, mathematics - see section 2). They were asked to what extent they agreed or disagreed with the definitions (RQ1) and which aspects should be specifically promoted in STEM education (RQ2). Not all participants reported their primary discipline. The results of those who did can be seen in Table 1. The responses were first qualitatively categorised inductively by the interdisciplinary project team with regard to key aspects addressed, and the number of mentions was recorded quantitatively. In a second step, the responses from computer scientists and non-computer scientists were contrasted by two scientists specialising in computer science education research.

To answer RQ3 and RQ4, the communication and development process involved in creating a simulation of forest ant movement for biology lessons was analysed as a case study. The purpose of the simulation is to enable empirical data collection on the relationship between leg movement type and the running speed of ants. The simulation was developed iteratively in Snap!, requiring intensive collaboration between the computer science team (computational modelling and implementation) and the biology education team (domain modelling and biology-specific didactic considerations).

Table 1. Overview of participants' backgrounds.

Discipline	n	Education research	Science	School
Biology	8	7	2	1
Chemistry	3	3	/	/
Computer Science	4	4	1	1
Mathematics	6	3	3	/
Physics	3	2	1	/
Overall	22	16	8	2
Some participants reported multiple fields or subjects. 'Overall' gives the value of unique participants in the corresponding category.				

For this investigation, the entire communication and development process, starting with the problem definition, technical clarifications, and the 15 prototypes that were created, was compiled and analysed as a dataset to examine both the underlying modelling processes and the modelling decisions that were made. The data were analysed using Mayring's qualitative content analysis [21], with an inductively developed category system.

First, the modelling decisions were identified and coded in a database together with relevant context information, which was present within the communication (occasion, motivation, decision-makers, reasons for decisions, context). This was done by sorting the communication and documentation chronologically and identifying modelling decisions. These were then cross-referenced with the prototypes.

The deductive codes were formed based on the main perspectives the respective stakeholders had during the development process: domain-specific (biology) and computational (CS-related). During the coding process, the categories of "usability" and "arbitrary" were identified inductively. Afterwards, the decisions were analysed with regard to dependency and categorised into "new" or "change to existing" decisions. Each decision (except the initial definition) was assigned a predecessor, or trigger, to recursively trace it back to the initial definitions/decisions. The resulting graph was analysed to gain further insight into the modelling processes.

4 Results

In this section, the evaluation results of the expert study (RQ1 and RQ2) are presented and contrasted with the findings from the case study (RQ3, italics). Finally, we present the results for RQ4.

4.1 Modelling in STEM Subjects: What Matters?

Modelling is a scientific and cyclical method. The evaluation of the expert study provided important insights for an interdisciplinary understanding of modelling. The definition of modelling as a scientific and cyclical method that is used for a specific purpose was endorsed overall. In particular, several experts from different disciplines explicitly

emphasised the cyclical nature of modelling as central; for example, one computer science expert noted, “Cyclical work is inherent in modelling”, while a biology expert commented that the definition “lacks the cyclicity of the concept of modelling, which could be emphasized more strongly”. Nevertheless, some participants (exclusively natural sciences and mathematics) expressed doubts as to whether a cyclical structure is necessarily required or whether linear processes are also possible.

The importance of modelling as a cyclical method finds support in the analysis of the case study (RQ3). The communication process involved in creating the simulation revealed a constant shift between biological and computational modelling decisions as an ongoing process. From the concretisation of the technical (biology didactic) requirements, to the continuous questioning of the “purposes” of modelling or simulation, to decisions made within the framework of what was feasible given time and resource constraints, a continuous interdisciplinary exchange based on the developed prototypes was necessary. Even if both subject-specific and computational decisions could have been made by a single person (with subject-specific and computational expertise), it would be expected that insights from the computational implementation of the subject-specific requirements would continuously lead to concretisation and adjustments. A linear approach, as suggested by some participants, is difficult to imagine in the development of a simulation in a non-professional context.

Modelling involves a product-oriented and process-oriented perspective. The distinction between the two perspectives was generally welcomed. However, there was also criticism of this separation: in particular, it was questioned whether the two perspectives are actually clearly distinct from each other in practice, as modelling and reflection often occur in close interplay. Accordingly, the importance of reflecting on the modelling process is emphasised in order to understand the limitations and quality of the model. Other experts, however, see reflection as less central, as they see it more as a consequence of the modelling process than a separate step.

The case study revealed a close interconnection between product-oriented and process-oriented perspectives due to the continuous need for reflection, with corresponding effects on modelling decisions. Of the 27 modelling decisions identified, 16 resulted from reflection and correction or concretisation of existing decisions. In the later cycles in particular, the proportion of revisions to modelling decisions made increased significantly compared to new decisions.

There is a need for clearer terminology. The expert study emphasised the importance of clear terminology for interdisciplinary understanding. Some participants found terms such as “analyse”, “apply” and “produce” unclear and would have liked a more precise description of the respective activities and process steps. Against the backdrop of interdisciplinarity, this poses a particular challenge: some of the experts noted that the generalised definition causes subject-specific methodological differences to be lost.

The terminology problem also became apparent during the analysis of communication in the case study, in which different understandings of terms, but also of methods, led to misunderstandings and, in some cases, frustration, which could only be overcome through compromise. In our case, communication posed a particular problem, as basic terms were used differently among the participating disciplines (e.g., simulation versus

animation) or were unfamiliar (“modelling technique”). In addition, the computational modelling and implementation of the biological models required them to be specified in detail, which had not previously been considered necessary from a technical perspective: “professional” simulations used in teaching specify model assumptions, but often do not make them clear and are therefore not questioned by either teachers or learners. This need for clear communication was in our case met, by using the prototypes as explicit examples to convey and discuss our ideas. The first few iterations show greater diversity. As the project progressed, the changes became more minor, as understanding of the final simulation converged.

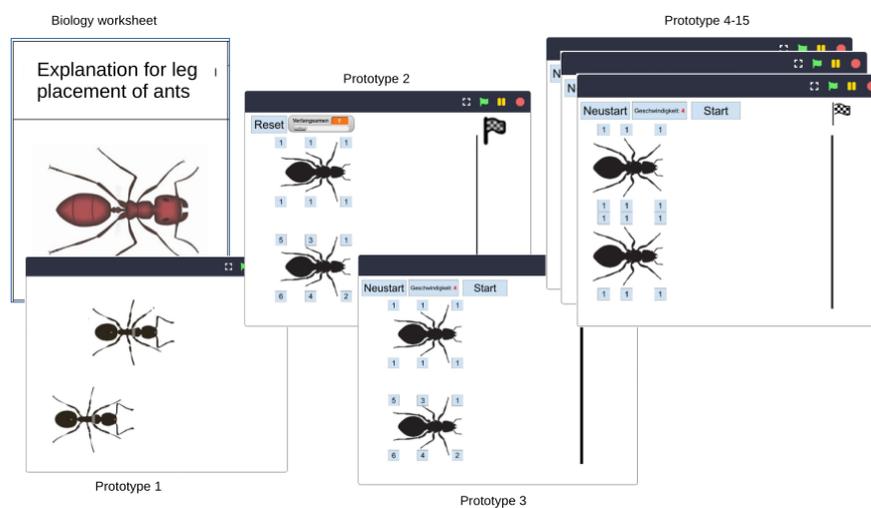


Fig. 1. Prototype changes during development.

In summary (RQ1), modelling is seen as a scientific method, as well as an abstraction for the sake of creating a product. The distinction between product-oriented and process-oriented perspectives is welcomed, as is the emphasis on cyclicity. We also identified a need for clearer terminology. These findings are supported by the case study (RQ3), where both cyclicity and terminology issues were clearly evident.

4.2 Modelling Competence: What Should be Promoted?

A reflective approach is important. Regarding which aspects should be prioritised in STEM education, the experts overwhelmingly emphasised the importance of a reflective approach. Students should not only be able to apply models, but also to critically question them and recognise their limitations and usefulness (reflection and a meta-level perspective). Particular emphasis was placed on the ability to interpret and evaluate, i.e., understanding whether a model is appropriate for a specific purpose and what insights can be derived from it. According to the experts, the ability to recognise models

as simplified and abstract representations of reality and to critically question this abstraction is particularly relevant. The understanding that models fundamentally involve simplifications and idealisations is also considered central.

Comparing these priorities with the interdisciplinary development of the simulation (RQ3) provides insight into what this can mean in practice. In the design and implementation process of the ant movement simulation, computational modelling skills proved to be key to reflecting on and evaluating the implemented domain model. For example, 11 modelling decisions were made from a computer science perspective, such as the division of movement dynamics into six time units. For informed model critique, learners may also need to understand the underlying computer science decisions. It seems reasonable to assume that going through this process independently could be a key experience for learners.

The role of models in science. Some experts explicitly point out that modelling competence should go beyond purely technical skills and should include, in particular, reflection on the role of models in knowledge acquisition processes. Models are thus understood not only as didactic media, to which they are often reduced, especially in science education, but as central epistemic instruments for gaining knowledge. This view underscores the important perspective of computer science in the creation of simulations as the “third pillar of science”.

The ambivalence described by the experts also played an important role in the clarification of the modelling purpose of our interdisciplinary discourse. On the one hand, the simulation was intended to enable students to independently formulate and test hypotheses for the purpose of gaining knowledge. On the other hand, in the lesson context, the simulation would also be used as a didactic medium, which, for biology education considerations and time, has already implemented almost all modelling decisions (without making them explicit). In order to strengthen the modelling skills of the learners, the idea is to enable learners to expand the simulation model in a knowledge-driven way, in which they can experience the purpose - modelling as implementation - and the associated modelling decisions.

Modelling may require perspective shifts. The ability to change perspectives was mentioned by some experts, especially with regard to conflicting goals (e.g., in the context of education for sustainable development). This competence enables a differentiated view of different fields of application and the handling of conflicting requirements for models.

In the case study, perspective shifts became necessary, for example, in the case of conflicting goals between accurate representation of reality and technical implementation in modelling the ant’s balance.

Furthermore, the competence to form hypotheses and test them empirically was also explicitly highlighted. In addition, the experts emphasised the importance of creativity as an essential component of modelling and as an important “future skill”. Manual skills and methodological knowledge, such as systems theory, mathematics, and programming, were also mentioned as helpful. It is worth mentioning here that a majority of experts see all aspects as relevant for support: “I don’t see any aspects that are not relevant in school”. This view is strongly represented especially among computer

science experts, be it through short, direct answers: “Everything is relevant” or a reproduction of the aspects contained in the definition.

In summary (RQ2), the central aspects to be promoted in science education are reflecting both on models, as well as modelling, as part of the process of knowledge acquisition.

4.3 Modelling Decisions in the Interdisciplinary Development of Simulations

This section examines how computational modelling is shaped by the interplay between computer science and domain-specific modelling decisions in the interdisciplinary development of simulations. The analysis of the modelling decisions made and their reasons during the development of the simulation revealed requirements for modelling expertise in the interdisciplinary development process. These can be divided into four categories (see Table 2).

So-called “domain-specific” modelling decisions (n=8) are motivated by the desire to increase the accuracy of the information to be transferred with respect to the modelling purpose. This purpose is formulated during the interdisciplinary preliminary specification. The simulation to be created thus has an initially defined content, or cargo that needs to be transferred [4]. Modelling decisions that directly serve this technical purpose of the simulation are called “domain-specific,” e.g., the decision to introduce a “slow leg speed” through which the movement of the ant can be better understood (purpose).

Decisions (n=11) were categorised as “computer science” decisions if they were motivated by computer science-related reasons for the implementation of the simulation (e.g., data structures, concrete implementations of algorithms), e.g., the storage of individual legs with the data structure “list”. This decision was primarily motivated by the practicability of the implementation.

Decisions in favour of the user-friendliness of the simulation were categorised as “usability” (n=5), e.g., “clear, easily recognizable finish line”.

Occasionally, pragmatic modelling decisions had to be made that could not be assigned to any of the other categories or were conditioned by other decisions (“arbitrary,” n=3), but had no independent motivation concerning the purpose, e.g., determining how exactly “adjustable” should be implemented concerning leg speed.

The analysis of the modelling decisions shows that their categorisation depends largely on the respective objective within the development process. A decision that is identical in content can be justified and classified differently depending on the motivation. This illustrates the close connection between modelling decisions and modelling competence, as the conscious handling of modelling objectives and their effects on implementation represents essential competencies in the modelling process.

For the acquisition of modelling competence, this means that learners must not only develop the ability to create models, but also to reflect on the objectives underlying their modelling decisions. In the case study, this was exemplified by the decision to use a three-stage setting for leg speed. This was initially made arbitrarily, but under different conditions, such as the availability of ready-made program modules, it would have been justified from a computer science (CS) perspective. Learners must therefore be

able to recognise different motivations for modelling decisions and reflect on their own decisions within a structured development process.

Moreover, the analysis showed that many modelling decisions were not determined by biology alone, but emerged in negotiation, often proposed from the CS side and then validated or adjusted from the biology side. This happened as part of iterative cycles in which the purpose of the simulation (What questions should the simulation answer?) was regularly challenged. This forced reflection and revision from both CS and biology. To summarise: CS and domain-specific (as well as usability and arbitrary) modelling decisions are dependent on each other and mutually trigger each other through reflection.

Table 2. Categories of modelling decisions with examples.

Domain specific	Computer science	Usability	Arbitrary
Those made to improve the model in relation to its specific purpose	Those made due to technical considerations and restrictions	Those made to improve the usability of the final simulation	Those made due to purely practical reasons, without the consideration of the purpose
...introduce a “slow leg-speed” through which the movement of the ant can be better understood	...the storage of individual legs as a list, due to ease of implementation	...clear, easily recognisable finish line	...three different leg speeds (because domain specific decision “variable leg speed” needs specific values)
8	11	5	3

5 Discussion

This research shows that integrating computational modelling and simulations into STEM education in schools has great potential to provide learners with a deeper understanding of scientific processes and interdisciplinary skills. Interdisciplinary collaboration clearly showed that both subject-matter education researchers and teachers often have an insufficient understanding of computational models and software development processes, and that basic computational terms and methods are often unknown or misunderstood. This deficit highlights the need for targeted support for developing computational skills, but also the challenges associated with this.

The development of the biology teaching simulation on ant locomotion not only highlighted the interdisciplinary challenges but also their potential in a school context: the cyclical modelling processes, with their continuous reflection on technical, computer science, and usability-oriented modelling decisions, led to a better understanding of simulations and the relevance of their underlying models among all participants. Although the ant simulation was successfully used in biology lessons, students were unable to gain deeper insights into the underlying computer science models and modelling

decisions due to a lack of computer science education classes. Future applications should therefore be accompanied by computer science lessons to give learners insights into what goes on “under the hood” – biology teachers were open and interested in this. In particular, questioning and independently developing simulations could lead to substantially stronger modelling competence.

Overall, the study showed that a comprehensive, interdisciplinary understanding of modelling and modelling skills is essential to realise the potential of computational modelling and simulations for STEM education. The challenges of interdisciplinary collaboration and the remaining educational gaps in the field of computational modelling open up important perspectives for future research and practical development. The goal should be to strengthen the technical and interdisciplinary skills of learners and teachers in the long term by integrating computer science and other STEM subjects more closely.

A number of teaching implications can be derived from the findings. From a science-propaedeutic perspective, simulations belong in the classroom: they are not only “given” tools to reproduce (established) content, but creative means for students to investigate their own questions about the world. To achieve this, students need to be given room for exploration in science classrooms while supported by experts. This support should come in the form of both domain-specific support as well as computer-science-related support. From teachers in particular, this requires the acquisition of foundational computational modelling competency. As this is not a given and cannot be assumed for all teachers, interdisciplinary cooperation between computer science education and other STEM subjects should be promoted and implemented.

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